Study guide: Finite difference schemes for diffusion processes

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Contents

1	The	1D diffusion equation
	1.1	The initial-boundary value problem for 1D diffusion
	1.2	Step 1: Discretizing the domain
	1.3	The discrete solution
	1.4	Step 2: Fulfilling the equation at the mesh points
	1.5	Step 3: Replacing derivatives by finite differences
	1.6	Step 4: Formulating a recursive algorithm
	1.7	The mesh Fourier number
	1.8	The finite difference stencil
	1.9	The computational algorithm for the Forward Euler scheme
	1.10	The Python implementation of the computational algorithm
	1.11	Moving finite difference stencil
	1.12	Demo program
	1.13	Forward Euler applied to an initial plug profile
		Forward Euler applied to a Gaussian profile
	1.15	Backward Euler scheme
	1.16	Let's write out the equations for $N_x = 3$
	1.17	Two classes of discretization methods: explicit and implicit
	1.18	The linear system for a general N_x
	1.19	A is very sparse: a tridiagonal matrix
	1.20	Detailed expressions for the matrix entries
		The right-hand side
	1.22	Naive Python implementation with a dense $(N_x + 1) \times (N_x + 1)$ matrix
		A sparse matrix representation will dramatically reduce the computational complexity
	1.24	Computing the sparse matrix
	1.25	Backward Euler applied to a plug profile
		Backward Euler applied to a Gaussian profile
	1.27	Crank-Nicolson scheme
	1 20	Averaging in time is necessary in the Crank Nicolan scheme

	1.29	Crank-Nicolsoon scheme written out	10
	1.30	Crank-Nicolson applied to a plug profile	11
	1.31	Crank-Nicolson applied to a Gaussian profile	11
	1.32	The θ rule	11
	1.33	The Laplace and Poisson equation	12
		We can solve 1D Poisson/Laplace equation by going to infinity in time-dependent	
		diffusion equations	12
	1.35	Extensions	12
2	Ana	lysis of schemes for the diffusion equation	13
	2.1	Properties of the solution	13
	2.2	Example	13
	2.3	Visualization of the damping in the diffusion equation	14
	2.4	Damping of a discontinuity; problem and model	14
	2.5	Damping of a discontinuity; Backward Euler simulation	15
	2.6	Damping of a discontinuity; Forward Euler simulation	15
	2.7	Damping of a discontinuity; Crank-Nicolson simulation	15
	2.8	Fourier representation	15
	2.9	Analysis of the finite difference schemes	15
	2.10	Analysis of the Forward Euler scheme	16
	2.11	Results for stability	16
		Analysis of the Backward Euler scheme	16
	2.13	Stability	16
	2.14	Analysis of the Crank-Nicolson scheme	17
	2.15	Stability	17
		Summary of accuracy of amplification factors; large time steps	19
	2.17	Summary of accuracy of amplification factors; time steps around the Forward Euler	
		stability limit	19
	2.18	Summary of accuracy of amplification factors; small time steps	19
		Observations	10

1 The 1D diffusion equation

The famous diffusion equation, also known as the heat equation, reads

$$\frac{\partial u}{\partial t} = \alpha \frac{\partial^2 u}{\partial x^2}$$

Here,

- u(x,t): unknown
- α: diffusion coefficient

Alternative, compact notation:

$$u_t = \alpha u_{xx}$$

2

1.1 The initial-boundary value problem for 1D diffusion

$$\frac{\partial u}{\partial t} = \alpha \frac{\partial^2 u}{\partial x^2}, \quad x \in (0, L), \ t \in (0, T]$$
 (1)

$$u(x,0) = I(x), \qquad x \in [0,L]$$

$$(2)$$

$$u(0,t) = 0, t > 0, (3)$$

$$u(L,t) = 0, t > 0. (4)$$

Note:

- First-order derivative in time: one initial condition
- Second-order derivative in space: a boundary condition at each point of the boundary (2 points in 1D)
- Numerous applications throughout physics and biology

1.2 Step 1: Discretizing the domain

Mesh in time:

$$0 = t_0 < t_1 < t_2 < \dots < t_{N_t - 1} < t_{N_t} = T$$

$$\tag{5}$$

Mesh in space:

$$0 = x_0 < x_1 < x_2 < \dots < x_{N_x - 1} < x_{N_x} = L \tag{6}$$

Uniform mesh with constant mesh spacings Δt and Δx :

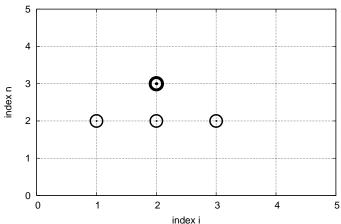
$$x_i = i\Delta x, \ i = 0, \dots, N_x, \quad t_i = n\Delta t, \ n = 0, \dots, N_t$$

$$(7)$$

1.3 The discrete solution

- The numerical solution is a mesh function: $u_i^n \approx u_e(x_i, t_n)$
- ullet Finite difference stencil (or scheme): equation for u_i^n involving neighboring space-time points





1.4 Step 2: Fulfilling the equation at the mesh points

Require the PDE (1) to be fulfilled at an arbitrary interior mesh point (x_i, t_n) leads to

$$\frac{\partial}{\partial t}u(x_i, t_n) = \alpha \frac{\partial^2}{\partial x^2}u(x_i, t_n) \tag{8}$$

Applies to all interior mesh points: $i = 1, ..., N_x - 1$ and $n = 1, ..., N_t - 1$

For n = 0 we have the initial conditions u = I(x) and $u_t = 0$

At the boundaries $i = 0, N_x$ we have the boundary condition u = 0.

1.5 Step 3: Replacing derivatives by finite differences

Use a forward difference in time and a centered difference in space (Forward Euler scheme):

$$[D_t^+ u = \alpha D_x D_x u]_i^n \tag{9}$$

Written out,

$$\frac{u_i^{n+1} - u_i^n}{\Delta t} = \alpha \frac{u_{i+1}^n - 2u_i^n + u_{i-1}^n}{\Delta x^2} \tag{10}$$

Initial condition: $u_i^0 = I(x_i), i = 0, 1, \dots, N_x$.

1.6 Step 4: Formulating a recursive algorithm

- Nature of the algorithm: compute u in space at $t = \Delta t, 2\Delta t, 3\Delta t, ...$
- \bullet Two time levels are involved in the general discrete equation: n+1 and n

• u_i^n is already computed for $i = 0, \ldots, N_x$, and u_i^{n+1} is the unknown quantity

Solve the discretized PDE for the unknown u_i^{n+1} :

$$u_i^{n+1} = u_i^n + Fo\left(u_{i+1}^n - 2u_i^n + u_{i-1}^n\right)$$
(11)

where

$$Fo = \alpha \frac{\Delta t}{\Delta x^2}$$

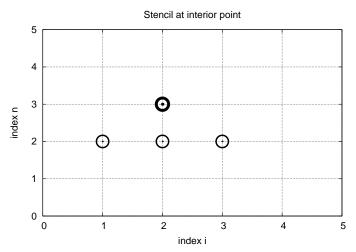
1.7 The mesh Fourier number

$$Fo = \alpha \frac{\Delta t}{\Delta x}$$

Observe.

There is only one parameter, Fo, in the discrete model: Fo lumps mesh parameters Δt and Δx with the only physical parameter, the diffusion coefficient α . The value Fo and the smoothness of I(x) govern the quality of the numerical solution.

1.8 The finite difference stencil



1.9 The computational algorithm for the Forward Euler scheme

5

1. compute $u_i^0 = I(x_i), i = 0, ..., N_x$

- 2. for $n = 0, 1, \dots, N_t$:
 - (a) compute u_i^{n+1} from (11) for all the internal spatial points $i=1,\ldots,N_x-1$
 - (b) set the boundary values $u_i^{n+1} = 0$ for i = 0 and $i = N_x$

Notice.

We visit one mesh point (x_i, t_{n+1}) at a time, and we have an explicit formula for computing the associated u_i^{n+1} value. The spatial points can be updated in any sequence, but the time levels t_n must be updated in cronological order: t_n before t_{n+1} .

1.10 The Python implementation of the computational algorithm

```
x = linspace(0, L, Nx+1)
                              # mesh points in space
dx = x[1] - x[0]
t = linspace(0, T, Nt+1)
                              # mesh points in time
dt = t[1] - t[0]
Fo = a*dt/dx**2
u = zeros(Nx+1)
u_1 = zeros(Nx+1)
# Set initial condition u(x,0) = I(x) for i in range(0, Nx+1):
    u 1[i] = I(x[i])
for n in range(0, Nt):
     # Compute u at inner mesh points
    for i in range(1, Nx):
         u[i] = u_1[i] + Fo*(u_1[i-1] - 2*u_1[i] + u_1[i+1])
    # Insert boundary conditions
    u[0] = 0; u[Nx] = 0
    # Update u_1 before next step
    u_1[:]= u
    # or more efficient switch of references
    #u_1, u = u, u_1
```

1.11 Moving finite difference stencil

web page¹ or a movie file².

1.12 Demo program

- Program: diffu1D_u0.py3
- Produces animation on the screen
- Each frame stored in tmp_frame%04d.png files tmp_frame0000.png, tmp_frame0001.png, ...

6

http://tinyurl.com/opdfafk/pub/mov-diffu/diffuID_PDE_FE_Dirichlet_stencil_gpl/index.html
http://tinyurl.com/opdfafk/pub/mov-diffu/diffuID_PDE_FE_Dirichlet_stencil_gpl/movie.ogg
http://tinyurl.com/mm5587k/diffu/diffID_u0.py

How to make movie file in modern formats:

```
Terminal> name=tmp_frame%04d.png
Terminal> fps=8 # frames per second in movie
Terminal> avconv -r $fps -i $name -vcodec flv
                                                   movie.flv
Terminal> avconv -r $fps -i $name -vcodec libx64
                                                   movie.mp4
Terminal> avconv -r $fps -i $name -vcodec libvpx
Terminal> avconv -r $fps -i $name -vcodec libtheora movie.ogg
```

1.13 Forward Euler applied to an initial plug profile

 $N_r = 50$. The method results in a growing, unstable solution if Fo > 0.5.

Choosing Fo = 0.5 gives a strange saw tooth-like curve.

Link to movie file⁴

Lowering Fo to 0.25 gives a smooth (expected) solution.

Link to movie file⁵

1.14 Forward Euler applied to a Gaussian profile

```
N_x = 50. Fo = 0.5.
   Link to movie file<sup>6</sup>
   Link to movie file<sup>7</sup>
```

1.15 Backward Euler scheme

Backward difference in time, centered difference in space:

$$[D_t^- u = D_x D_x u]_i^n \tag{12}$$

Written out:

$$\frac{u_i^n - u_i^{n-1}}{\Delta t} = \alpha \frac{u_{i+1}^n - 2u_i^n + u_{i-1}^n}{\Delta x^2}$$
(13)

Assumption: u_i^{n-1} is computed, but all quantities at the new time level t_n are unknown.

Notice.

We cannot solve wrt u_i^n because that unknown value is coupled to two other unknown values: u_{i-1}^n and u_{i+1}^n . That is, all the new unknown values are coupled to each other in a linear system of algebraic equations.

1.16 Let's write out the equations for $N_x = 3$

Equation (13) written for i = 1, ..., Nx - 1 = 1, 2 becomes

$$\begin{split} \frac{u_1^n - u_1^{n-1}}{\Delta t} &= \alpha \frac{u_2^n - 2u_1^n + u_0^n}{\Delta x^2} \\ \frac{u_2^n - u_2^{n-1}}{\Delta t} &= \alpha \frac{u_3^n - 2u_2^n + u_1^n}{\Delta x^2} \end{split} \tag{14}$$

$$\frac{u_2^n - u_2^{n-1}}{\Delta t} = \alpha \frac{u_3^n - 2u_2^n + u_1^n}{\Delta x^2}$$
(15)

(The boundary values u_0^n and u_3^n are known as zero.)

Collecting the unknown new values on the left-hand side and writing as 2×2 matrix system:

$$\left(\begin{array}{cc} 1+2Fo & -Fo \\ -Fo & 1+2Fo \end{array} \right) \left(\begin{array}{c} u_1^n \\ u_2^n \end{array} \right) = \left(\begin{array}{c} u_1^{n-1} \\ u_2^{n-1} \end{array} \right)$$

1.17 Two classes of discretization methods: explicit and implicit

Implicit.

Discretization methods that lead linear systems are known as implicit methods.

Explicit.

Discretization methods that avoid linear systems and have an explicit formula for each new value of the unknown are called explicit methods.

The linear system for a general N_r

$$-F_o u_{i-1}^n + (1+2F_o) u_i^n - F_o u_{i+1}^n = u_{i-1}^{n-1}$$
(16)

for i = 1, ..., Nx - 1.

What are the unknowns in the linear system?

- 1. either u_i^n for $i = 1, ..., N_x 1$ (all internal spatial mesh points)
- 2. or u_i^n , $i = 0, \ldots, N_x$ (all spatial points)

The linear system in matrix notation:

$$AU = b, \quad U = (u_0^n, \dots, u_N^n)$$

⁴http://tinyurl.com/opdfafk/pub/mov-diffu/diffu1D_u0_FE_plug/movie.ogg

⁵http://tinyurl.com/opdfafk/pub/mov-diffu/diffu1D_u0_FE_plug_Fo025/movie.ogg

⁶http://tinyurl.com/opdfafk/pub/mov-diffu/diffu1D_u0_FE_gaussian1/movie.ogg

⁷http://tinyurl.com/opdfafk/pub/mov-diffu/diffu1D_u0_FE_plug_gaussian2/movie.ogg

1.19 A is very sparse: a tridiagonal matrix

$$A = \begin{pmatrix} A_{0,0} & A_{0,1} & 0 & \cdots & \cdots & \cdots & \cdots & 0 \\ A_{1,0} & A_{1,1} & 0 & \ddots & & & \vdots \\ 0 & A_{2,1} & A_{2,2} & A_{2,3} & \ddots & & & \vdots \\ \vdots & \ddots & \ddots & \ddots & \ddots & \ddots & & \vdots \\ \vdots & & \ddots & \ddots & \ddots & \ddots & \ddots & \vdots \\ \vdots & & & 0 & A_{i,i-1} & A_{i,i} & A_{i,i+1} & \ddots & \vdots \\ \vdots & & & \ddots & \ddots & \ddots & \ddots & 0 \\ \vdots & & & & \ddots & \ddots & \ddots & \ddots & 0 \\ \vdots & & & & \ddots & \ddots & \ddots & \ddots & 0 \\ \vdots & & & & \ddots & \ddots & \ddots & \ddots & A_{N_x-1,N_x} \\ 0 & \cdots & \cdots & \cdots & \cdots & 0 & A_{N_x,N_x-1} & A_{N_x,N_x} \end{pmatrix}$$

$$(17)$$

1.20 Detailed expressions for the matrix entries

The nonzero elements are given by

$$A_{i,i-1} = -F_o \tag{18}$$

$$A_{i,i} = 1 + 2F_o (19)$$

$$A_{i,i+1} = -F_o$$
 (20)

for $i = 1, ..., N_x - 1$.

The equations for the boundary points correspond to

$$A_{0,0} = 1$$
, $A_{0,1} = 0$, $A_{N_{\tau},N_{\tau}-1} = 0$, $A_{N_{\tau},N_{\tau}} = 1$

1.21 The right-hand side

$$b = \begin{pmatrix} b_0 \\ b_1 \\ \vdots \\ b_i \\ \vdots \\ b_{N-} \end{pmatrix}$$
 (21)

with

$$b_0 = 0 (22)$$

$$b_i = u_i^{n-1}, \quad i = 1, \dots, N_x - 1$$
 (23)

$$b_{N_{-}} = 0$$
 (24)

1.22 Naive Python implementation with a dense $(N_x+1)\times(N_x+1)$ matrix

x = linspace(0, L, Nx+1) # mesh points in space dx = x[1] - x[0]t = linspace(0, T, N+1)# mesh points in time u = zeros(Nx+1) $u_1 = zeros(Nx+1)$ # Data structures for the linear system A = zeros((Nx+1, Nx+1))b = zeros(Nx+1)for i in range(1, Nx): A[i,i-1] = -Fo A[i,i+1] = -Fo A[i,i] = 1 + 2*FoA[0,0] = A[Nx,Nx] = 1# Set initial condition u(x,0) = I(x)for i in range(0, Nx+1): $u_1[i] = I(x[i])$ import scipy.linalg for n in range(0, Nt): # Compute b and solve linear system for i in range(1, Nx): $b[i] = -u_1[i]$ b[0] = b[Nx] = 0u[:] = scipy.linalg.solve(A, b) # Update u_1 before next step u_1, u = u, u_1

1.23 A sparse matrix representation will dramatically reduce the computational complexity

- With a dense matrix, the algorithm leads to $\mathcal{O}(N_x^3)$ operations
- Utilizing the sparsity, the algorithm has complexity $\mathcal{O}(N_x)$!
- scipy.sparse enables storage and calculations with the three nonzero diagonals only

```
# Representation of sparse matrix and right-hand side
diagonal = zeros(Nx+1)
lower = zeros(Nx)
upper = zeros(Nx)
b = zeros(Nx+1)
```

1.24 Computing the sparse matrix

```
# Precompute sparse matrix
diagonal[:] = 1 + 2*Fo
lower[:] = -Fo #1
upper[:] = -Fo #1
# Insert boundary conditions
diagonal[0] = 1
upper[0] = 0
```

```
diagonal[Nx] = 1
lower[-1] = 0
import scipy.sparse
A = scipy.sparse.diags(
    diagonals=[main, lower, upper],
    offsets=[0, -1, 1], shape=(Nx+1, Nx+1),
    format='csr')

# Set initial condition
for i in range(0, Nx+1):
    u_1[i] = I(x[i])

for n in range(0, Nt):
    b = u_1
    b[0] = b[-1] = 0.0 # boundary conditions
    u[:] = scipy.sparse.linalg.spsolve(A, b)
    # Switch variables before next step
    u_1, u = u, u_1
```

1.25 Backward Euler applied to a plug profile

$$N_x = 50$$
. $Fo = 0.5$.
Link to movie file⁸

1.26 Backward Euler applied to a Gaussian profile

$$\begin{split} N_x &= 50. \\ \text{Link to movie file}^9 \\ Fo &= 5. \\ \text{Link to movie file}^{10} \end{split}$$

1.27 Crank-Nicolson scheme

The PDE is sampled at points $(x_i, t_{n+\frac{1}{2}})$ (at the spatial mesh points, but in between two temporal mesh points).

$$\frac{\partial}{\partial t}u(x_i,t_{n+\frac{1}{2}})=\alpha\frac{\partial^2}{\partial x^2}u(x_i,t_{n+\frac{1}{2}})$$

for $i = 1, ..., N_x - 1$ and $n = 0, ..., N_t - 1$.

Centered differences in space and time:

$$[D_t u = \alpha D_x D_x u]_i^{n + \frac{1}{2}}$$

1.28 Averaging in time is necessary in the Crank-Nicolson scheme

Right-hand side term:

$$\frac{1}{\Delta x^2} \left(u_{i-1}^{n+\frac{1}{2}} - 2 u_i^{n+\frac{1}{2}} + u_{i+1}^{n+\frac{1}{2}} \right)$$

Problem: $u_i^{n+\frac{1}{2}}$ is not one of the unknowns we compute.

Solution: replace $u_i^{n+\frac{1}{2}}$ by an arithmetic average:

$$u_i^{n+\frac{1}{2}} \approx \frac{1}{2} \left(u_i^n + u_i^{n+1} \right)$$

In compact notation (arithmetic average in time \overline{u}^t):

$$[D_t u = \alpha D_x D_x \overline{u}^t]_i^{n + \frac{1}{2}}$$

1.29 Crank-Nicolsoon scheme written out

$$u_{i}^{n+1} - \frac{1}{2}Fo(u_{i-1}^{n+1} - 2u_{i}^{n+1} + u_{i+1}^{n+1}) = u_{i}^{n} + \frac{1}{2}Fo(u_{i-1}^{n} - 2u_{i}^{n} + u_{i+1}^{n})$$
 (25)

Observe:

- The unknowns are $u_{i-1}^{n+1}, u_i^{n+1}, u_{i+1}^{n+1}$
- These unknowns are coupled to each other (in a linear system)
- Must solve AU = b at each time level

Now,

$$A_{i,i-1} = -\frac{1}{2}F_o (26)$$

$$A_{i,i} = \frac{1}{2} + F_o (27)$$

$$F_{i,i+1} = -\frac{1}{2}F_o$$
 (28)

for internal points. For boundary points,

$$A_{0,0} = 1$$
 (29)

$$A_{0,1} = 0 (30)$$

$$A_{N_x,N_x-1} = 0 (31)$$

$$A_{N_{\tau},N_{\tau}} = 1 \tag{32}$$

Right-hand side:

$$b_0 = 0 (33)$$

$$b_i = u_i^{n-1}, \quad i = 1, \dots, N_x - 1$$
 (34)

$$\rho_{N_x} = 0 \tag{35}$$

 $^{^{8}} http://tinyurl.com/opdfafk/pub/mov-diffu/diffu1D_u0_BE_plug/movie.ogg$ $^{9} http://tinyurl.com/opdfafk/pub/mov-diffu/diffu1D_u0_BE_gaussian1/movie.ogg$

¹⁰ http://tinyurl.com/opdfafk/pub/mov-diffu/diffu1D_u0_BE_gaussian1_Fo5/movie.ogg

1.30 Crank-Nicolson applied to a plug profile

Crank-Nicolson never blows up, so any Fo can be used (modulo loss of accuracy).

 $N_x = 50$. Fo = 5 gives instabilities.

Link to movie file 11

 $N_x = 50$. Fo = 0.5 gives a smooth solution.

Link to movie file¹²

1.31 Crank-Nicolson applied to a Gaussian profile

 $N_x = 50.$

Link to movie file¹³

Fo = 5.

Link to movie file¹⁴

1.32 The θ rule

The θ rule condenses a family of finite difference approximations in time to one formula

- $\theta = 0$ gives the Forward Euler scheme in time
- $\theta = 1$ gives the Backward Euler scheme in time
- $\theta = \frac{1}{2}$ gives the Crank-Nicolson scheme in time

Applied to $u_t = \alpha u_{xx}$:

$$\frac{u_i^{n+1} - u_i^n}{\Delta t} = \alpha \left(\theta \frac{u_{i+1}^{n+1} - 2u_i^{n+1} + u_{i-1}^{n+1}}{\Delta x^2} + (1 - \theta) \frac{u_{i+1}^n - 2u_i^n + u_{i-1}^n}{\Delta x^2} \right)$$

Matrix entries:

$$A_{i,i-1} = -F_o\theta$$
, $A_{i,i} = 1 + 2F_o\theta$, $A_{i,i+1} = -F_o\theta$

Right-hand side:

$$b_i = u_i^n + F_o(1 - \theta) \frac{u_{i+1}^n - 2u_i^n + u_{i-1}^n}{\Delta x^2}$$

1.33 The Laplace and Poisson equation

Laplace equation:

$$\nabla^2 u = 0$$
, 1D: $u''(x) = 0$

Poisson equation:

$$-\nabla^2 u = f$$
, 1D: $-u''(x) = f(x)$

These are limiting behavior of time-dependent diffusion equations if

$$\lim_{t \to \infty} \frac{\partial u}{\partial t} = 0$$

Then $u_t = \alpha u_{xx} + 0$ in the limit $t \to \infty$ reduces to

$$u_{xx} + f = 0$$

1.34 We can solve 1D Poisson/Laplace equation by going to infinity in time-dependent diffusion equations

Looking at the numerical schemes, $Fo \to \infty$ leads to the Laplace or Poisson equations (without f or with f, resp.).

Good news: choose Fo large in the BE or CN schemes and one time step is enough to produce the stationary solution for $t \to \infty$.

1.35 Extensions

These extensions are performed exactly as for a wave equation as they only affect the spatial derivatives (which are the same as in the wave equation).

- Variable coefficients
- Neumann and Robin conditions
- 2D and 3D

Future versions of this document will for completeness and independence of the wave equation document feature info on the three points. The Robin condition is new, but straightforward to handle:

$$-\alpha \frac{\partial u}{\partial n} = h_T(u - U_s), \quad [-\alpha D_x u = h_T(u - U_s)]_i^n$$

2 Analysis of schemes for the diffusion equation

2.1 Properties of the solution

The PDE

$$u_t = \alpha u_{xx} \tag{36}$$

admits solutions

$$u(x,t) = Qe^{-\alpha k^2 t} \sin(kx) \tag{37}$$

Observations from this solution:

- The initial shape $I(x) = Q \sin kx$ undergoes a damping $\exp(-\alpha k^2 t)$
- The damping is very strong for short waves (large k)
- The damping is weak for long waves (small k)
- ullet Consequence: u is smoothened with time

¹¹http://tinyurl.com/opdfafk/pub/mov-diffu/diffu1D_u0_theta_plug_Fo5/movie.ogg

¹²http://tinyurl.com/opdfafk/pub/mov-diffu/diffu1D_u0_theta_plug/movie.ogg

¹³ http://tinyurl.com/opdfafk/pub/mov-diffu/diffu1D_u0_theta_gaussian1/movie.ogg

¹⁴http://tinyurl.com/opdfafk/pub/mov-diffu/diffu1D_u0_theta_gaussian1_Fo5/movie.ogg

2.2 Example

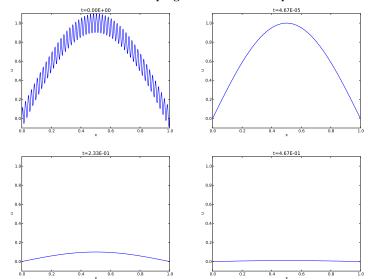
Test problem:

$$\begin{array}{ll} u_t = u_{xx}, & x \in (0,1), \ t \in (0,T] \\ u(0,t) = u(1,t) = 0, & t \in (0,T] \\ u(x,0) = \sin(\pi x) + 0.1\sin(100\pi x) \end{array}$$

Exact solution:

$$u(x,t) = e^{-\pi^2 t} \sin(\pi x) + 0.1e^{-\pi^2 10^4 t} \sin(100\pi x)$$
(38)

2.3 Visualization of the damping in the diffusion equation



2.4 Damping of a discontinuity; problem and model

Problem

Two pieces of a material, at different temperatures, are brought in contact at t=0. Assume the end points of the pieces are kept at the initial temperature. How does the heat flow from the hot to the cold piece?

Solution.

Assume a 1D model is sufficient (insulated rod):

$$u(x,0) = \begin{cases} U_L, & x < L/2 \\ U_R, & x \ge L/2 \end{cases}$$

$$\frac{\partial u}{\partial t} = \alpha \frac{\partial^2 u}{\partial x^2}, \quad u(0,t) = U_L, \ u(L,t) = U_R$$

2.5 Damping of a discontinuity; Backward Euler simulation

 Movie^{15}

2.6 Damping of a discontinuity; Forward Euler simulation

 $Movie^{16}$

2.7 Damping of a discontinuity; Crank-Nicolson simulation

 $\rm Movie^{17}$

2.8 Fourier representation

Represent I(x) as a Fourier series

$$I(x) \approx \sum_{k \in K} b_k e^{ikx} \tag{39}$$

The corresponding sum for u is

$$u(x,t) \approx \sum_{k \in K} b_k e^{-\alpha k^2 t} e^{ikx}$$
 (40)

Such solutions are also accepted by the numerical schemes, but with an amplification factor A different from $\exp{(-\alpha k^2 t)}$:

$$u_q^n = A^n e^{ikq\Delta x} = A^n e^{ikx} \tag{41}$$

2.9 Analysis of the finite difference schemes

Stability:

- |A| < 1: decaying numerical solutions (as we want)
- A < 0: oscillating numerical solutions (as we do not want)

Accuracy:

• Compare numerical and exact amplification factor: A vs $A_e = \exp(-\alpha k^2 \Delta t)$

¹⁵ http://tinyurl.com/opdfafk/pub/mov-diffu/BE_CO.5/index.html

¹⁶http://tinyurl.com/opdfafk/pub/mov-diffu/FE_CO.5/index.html

¹⁷ http://tinyurl.com/opdfafk/pub/mov-diffu/CN_C5/index.html

2.10 Analysis of the Forward Euler scheme

$$[D_t^+ u = \alpha D_x D_x u]_q^n$$

Inserting

$$u_q^n = A^n e^{ikq\Delta x}$$

leads to

$$A = 1 - 4C\sin^2\left(\frac{k\Delta x}{2}\right), \quad C = \frac{\alpha\Delta t}{\Delta x^2}$$
 (42)

The complete numerical solution is

$$u_q^n = (1 - 4C\sin^2 p)^n e^{ikq\Delta x}, \quad p = k\Delta x/2 \tag{43}$$

2.11 Results for stability

We always have $A \leq 1$. The condition $A \geq -1$ implies

$$4C\sin^2 p \le 2$$

The worst case is when $\sin^2 p = 1$, so a sufficient criterion for stability is

$$C \le \frac{1}{2} \tag{44}$$

or:

$$\Delta t \le \frac{\Delta x^2}{2\alpha} \tag{45}$$

Implications of the stability result.

Less favorable criterion than for $u_{tt}=c^2u_{xx}$: halving Δx implies time step $\frac{1}{4}\Delta t$ (not just $\frac{1}{2}\Delta t$ as in a wave equation). Need very small time steps for fine spatial meshes!

2.12 Analysis of the Backward Euler scheme

$$[D_t^- u = \alpha D_x D_x u]_q^n$$

$$u_q^n = A^n e^{ikq\Delta x}$$

$$A = (1 + 4C\sin^2 p)^{-1} \tag{46}$$

$$u_q^n = (1 + 4C\sin^2 p)^{-n} e^{ikq\Delta x}$$
(47)

2.13 Stability

We see from (46) that |A| < 1 for all $\Delta t > 0$ and that A > 0 (no oscillations).

2.14 Analysis of the Crank-Nicolson scheme

The scheme

$$[D_t u = \alpha D_x D_x \overline{u}^x]_q^{n + \frac{1}{2}}$$

leads to

$$A = \frac{1 - 2C\sin^2 p}{1 + 2C\sin^2 p} \tag{48}$$

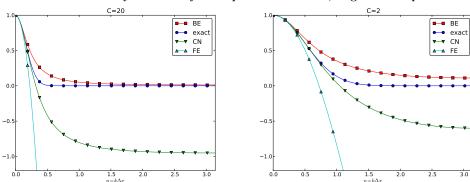
$$u_q^n = \left(\frac{1 - 2C\sin^2 p}{1 + 2C\sin^2 p}\right)^n e^{ikp\Delta x} \tag{49}$$

2.15 Stability

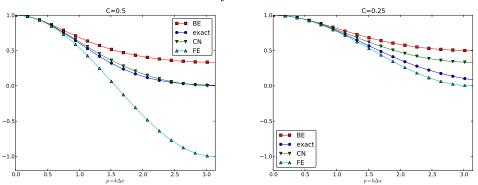
The criteria A>-1 and A<1 are fulfilled for any $\Delta t>0.$



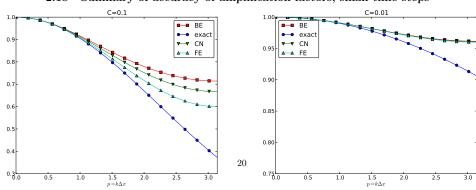
2.16 Summary of accuracy of amplification factors; large time steps



2.17 Summary of accuracy of amplification factors; time steps around the Forward Euler stability limit



2.18 Summary of accuracy of amplification factors; small time steps



2.19 Observations

ullet Crank-Nicolson gives oscillations and not much damping of short waves for increasing C.

- These waves will manifest themselves as high frequency oscillatory noise in the solution.
- All schemes fail to dampen short waves enough

The problems of correct damping for $u_t=u_{xx}$ is partially manifested in the similar time discretization schemes for $u'(t)=-\alpha u(t)$.

Index

diffusion equation, 1D, 1
heat equation, 1D, 1
mesh
finite differences, 2
mesh function, 2
stencil
1D diffusion equation, 2